POWDER DIFFRACTION BEAMLINE FOR *IN SITU* STUDIES OF STRUCTURAL AND CHEMICAL TRANSFORMATIONS (IXD)

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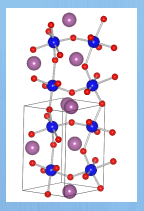
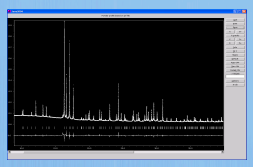
BROOKHAVEN NATIONAL LABORATORY

NATIONAL SYNCHROTRON LIGHT SOURCE II planned by Photon Sciences Directorate

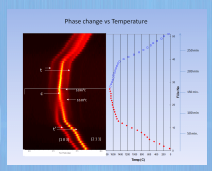
TECHNIQUES AND CAPABILITIES

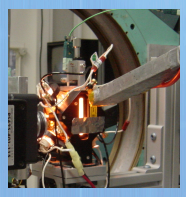
- IXD is a sagittal focused powder diffraction beamline on a TPW port, with continuously tunable x-ray energy from 5 to 25 keV.
- Powder crystallography, including solving and refining crystal structures, quantitative analysis of phase fraction and size/strain analysis.
- *In situ* powder-diffraction measurements to study, with sub-minute time resolution, the structural, morphological and chemical transformations in materials following changes in temperature (10K to 2000K), pressure, reaction gas flow and charging states.
- Anomalous (or resonant) x-ray diffraction studies by tuning the x-ray wavelength near the absorption edges in order to distinguish neighboring elements and oxidation states.
- Diffraction at grazing incidence and reflectivity.
- Residual, thermal and growth-stress measurements.





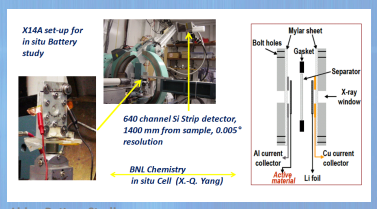
Monoclinic $ScMnO_3$: A New Multiferroic Material



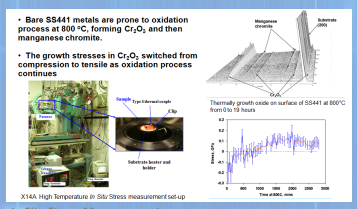


Quadrupole lamp furnace, up to 2000 K

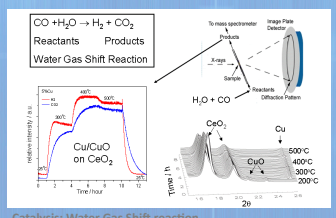
APPLICATIONS



Li-ion Battery Studies



In Situ Stress Measurement



Catalysis: Water Gas Shift reaction

In Situ X-ray Powder Diffraction Studies on Li-ion Battery Materials

One of the major science drivers for the proposed IXD beam line is to continue and enhance the current cutting-edge Li-ion battery studies at the NSLS. Lithium-ion batteries are the most promising candidate for use in hybrid electric vehicles (HEVs) and plug-in hybrid electric vehicles (PHEVs). Research topics in this field include the structure and morphology transformations in cathode materials during charge/ discharge processes, kinematics of chemical Lithium extraction, and *in situ* processing and synthesis of battery materials.

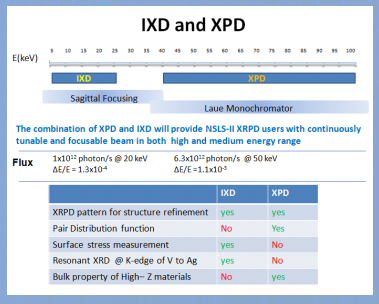
In Situ Surface Stress Analyses of High Temperature Alloys

High-temperature alloys have many important industrial applications in assuring a better performance of fossil-energy systems. Such alloy systems usually have multicomponent structures that undergo complicated physical and chemical processes in their surfaces in high temperature processes. New stress analyses method will be developed at IXD to simultaneously monitor the phase growth and the evolution of stress.

Real-Time Catalysis: *In-Situ* Structural Studies for Producing and Storing Hydrogen Fuel

Catalysis is the most critical field for sustainable energy production. Since real catalysts and catalytic processes are extremely complex, the availability of techniques for the real time characterization of catalytic systems as they evolve in time with a changing chemical environment is a high priority. The *in-situ* XRD capability of the IXD beamline affords the effective solution to such research needs, and will ensure the continuity of service to existing user groups.

SPECIFIC PROJECTS / ADDITIONAL INFORMATION



	IXD	XPD
XRPD pattern for structure refinement	yes	yes
Pair Distribution function	No	Yes
Surface stress measurement	yes	No
Resonant XRD @ K-edge of V to Ag	yes	No
Bulk property of High– Z materials	No	yes

- IXD aims to satisfy the practical needs for *ex situ* and *in situ* XRPD measurements by a wide user community, such as the user groups conducting studies on batteries, fuel cells, catalysis, high-temperature materials, light-metal production, and other energy industry-related and EERE-sponsored researchers.
- The medium x-ray energy range of IXD is in complementary to the already funded high energy (> 40 keV) x-ray powder diffraction beamline XPD.
- The High Temperature Materials Laboratory (HTML) at Oak Ridge National Laboratory is a DOE User Facility dedicated to solving materials problems that limit the efficiency and reliability of systems for power generation and energy conversion, distribution, and use. HTML supports the proposed IXD beamline and will join with other EERE-sponsored programs to pursue support from within EERE for scientific personnel and instruments in operating the IXD.
- IXD will work with the *Industrial User Program* of the Photon Science Directorate to explore new opportunities in industrial applications using synchrotron radiation.